

17 Gauss Way	Berkeley, CA 94720-5070	p: 510.642.0143	f: 510.642.8609	www.msri.org	
NOTETAKER CHECKLIST FORM					
(Complete one for each talk.)					
Name: Or;	Katz	_ Email/Phone:	ORIKA	TZ.OK@gmail.con	1
Speaker's Name:	Vered Rom	Kedar			
Talk Title: On	some me	apply re	parable	impact systems	
Date: <u>8 / 10 / 18</u> Time: <u>9 : 30 am</u> / pm (circle one)					
Please summarize the lecture in 5 or fewer sentences: Nar integrability, usually associated with smooth perturbing of smooth systems, is extended to a rich class of Hamiltonian					
impart systems, in which the impacts respect the symmetries of the underlying					
For sime of these VAM there may be applied Other simple impact instear buse					
inherently 1	non-rotatio nal not	ion - Rom Kedar	shows cases	s of notion conjugate to	
geodesic flow	on a flat torus wi	th several h	andles.		

CHECK LIST

(This is NOT optional, we will not pay for incomplete forms)

- Introduce yourself to the speaker prior to the talk. Tell them that you will be the note taker, and that you will need to make copies of their notes and materials, if any.
- Obtain ALL presentation materials from speaker. This can be done before the talk is to begin or after the talk; please make arrangements with the speaker as to when you can do this. You may scan and send materials as a .pdf to yourself using the scanner on the 3rd floor.
 - >• <u>Computer Presentations</u>: Obtain a copy of their presentation
 - Overhead: Obtain a copy or use the originals and scan them
 - <u>Blackboard</u>: Take blackboard notes in black or blue PEN. We will NOT accept notes in pencil or in colored ink other than black or blue.
 - Handouts: Obtain copies of and scan all handouts
- For each talk, all materials must be saved in a single .pdf and named according to the naming convention on the "Materials Received" check list. To do this, compile all materials for a specific talk into one stack with this completed sheet on top and insert face up into the tray on the top of the scanner. Proceed to scan and email the file to yourself. Do this for the materials from each talk.
- When you have emailed all files to yourself, please save and re-name each file according to the naming convention listed below the talk title on the "Materials Received" check list. (YYYY.MM.DD.TIME.SpeakerLastName)
- □ Email the re-named files to <u>notes@msri.org</u> with the workshop name and your name in the subject line.



MSRI workshop

October 2018

On some nearly separable impact systems

M. Pnueli and V. Rom-Kedar & The ISSI team: L. Becker, S. Elliott, B. Firester, S. Gonen Cohen

Previous related works:

Chemical reactions as a Hamiltonian impact system: L. Lerman & VR-K SIAM J. Appl. Dyn. Syst., Vol. 11, No. 1, pp. 416–446, 2012

Soft impacts theory and multi-dimensional chem reactions: M. Kloc & VR-K *SIAM J. Appl. Dyn. Syst.*, 13-3 (2014), pp. 1033-1059

Soft Billiards theory and non-ergodicity of such systems: W Turaev (1997-2012), w A. Rapoport 2006-2008)

Global behavior of nonlinear Hamiltonian dynamics for n>=2 d.o.f. :

Smooth integrable Hamiltonians:

energy momentum-bifurcation diagrams & Fomenko graphs

Near integrable Hamiltonians

KAM, separatrix splittings, resonances, parabolic resonances, Arnold diffusion..

Slow fast systems

Integrable/ergodic structure of subsystems, adiabatic invariants and their "jumps"

Billiards, Soft billiards, Oscillating billiards

ergodicity and its loss by singular perturbation theory, Fermi acceleration, equilibration

Impact systems and soft impact systems

- 1) far from integrable
- 2) close to integrable
- 3) close to ?

Content:

- Tri-atomic reactions and soft impact systems
- Main results I+II
- Near vertical walls (I)
- Near right angled corners (II)
- Summary, some open problems

Classical atom-diatom reactions:



How are the reaction rates related to detailed molecular models?

The Bohn-Oppenheimer Approximation –average over the electrons motion

$$H(r_A, r_B, r_C) = \sum \frac{p_i^2}{2m_i} + U(r_A - r_B, r_B - r_C, r_A - r_C)$$

Potential Energy Surface (PES)

3 body problem - the classical dynamics is chaotic !

Transition State Theory (TST) reduce to a 1 dof system along the "reaction coordinate"

Tri-atomic co-linear reactions

 $A+BC \rightarrow AB+C$ on a line (London, Eyring, Polanyi and Sato, 1930-1960's) :



Adiabatic approximation – 2 d.o.f system:

$$H(r_A, r_B, r_C) = \sum_{i=A, B, C} \frac{p_i^2}{2m_i} + U(r_A - r_B, r_B - r_C, (r_A - r_B) + (r_B - r_C))$$

Reaction mass-weighted coordinates (see, e.g. Tannor 06):

$$H(q, p) = \sum_{i=1,2} \frac{p_i^2}{2} + V_r(q_1, q_2), \quad q_2 = b(m) \sin \beta(m) r_{BC}$$

Product mass-weighted coordinates:

$$H(Q,P) = \sum_{i=1,2}^{\infty} \frac{P_i^2}{2} + V_p(Q_1,Q_2), \quad Q_1 = a(m)\sin\beta(m)r_{AB}$$

Mass weighted Jacobi co-ordinates:



A saddle in a corner

L. Lerman & V. R-K, SIAM DS 2012

$$H = \frac{p^2}{2} + aV_{local}(q) + bV_b(q;\varepsilon) + cV_{farfield}(q;\varepsilon)$$

- A : symmetric matrix with one positive and one negative eigenvalues
- **V**_b: A billiard-like potential limiting to a corner, e.g. $V_{exp}(q, \varepsilon) = \exp(-q_2/\varepsilon) + \exp((q_2 cq_1)/\varepsilon)$





A saddle in a corner

L. Lerman & V. R-K, SIAM DS 2012

$$H = \frac{p^2}{2} + a(q - q_s)^T A(q - q_s) + bV_b(q;\varepsilon) + cV_{farfield}(q;\varepsilon)$$

- A : symmetric matrix with one positive and one negative eigenvalues
- **V**_b: A billiard-like potential limiting to a corner, e.g. $V_{exp}(q, \varepsilon) = \exp(-q_2/\varepsilon) + \exp((q_2 cq_1)/\varepsilon)$





Qualitative behavior I – closeness results

(Kloc & RK, SIAM DS 2014)

Theorem (reflections) : ~ Given a billiard-like potential family $V(q;\epsilon)$ and a smooth bounded potential U(q), for a finite number of regular reflections, away from the boundary, the trajectories of the smooth Hamiltonian:

$$H = \frac{1}{2}p^2 + U(q) + V_b(q;\varepsilon),$$

limit, smoothly (C^r w.r.t. initial conditions), to the impact trajectories. Similarly, near tangent reflections, the limit is achieved in the C⁰ topology.

proof is very similar to the billiard case [Rapoport, RK and Turaev, Com Math Phys 07]



Qualitative behavior II – when does TST work?

L. Lerman & V. R-K, SIAM DS 2012

Conjecture: When ω/λ is smaller than δ (a known geometrical factor)



 $\beta = \pi/3, L = 6, 26, 46, ..., 206, u_s = (2.5, 0.3).$

Qualitative behavior III – can stable tri-atomic periodic configurations emerge?





YES! Near symmetric p.o. of the impact system! (continuation in ε at fixed Floquet multipliers):



Content:

- Tri-atomic reactions and far from integrable soft impact systems
- Main results I+II
- Near vertical walls (I)
- Near right angled corners (II)
- Summary, open problems

Mechanical examples of near-integrable impact system:



C^r smooth coupling



tilted wall



C^r smooth boundary deformation



coupling and deformation



Take home message:

We extend the existing perturbation theory to a much larger class of problems

We show that new phenomena emerge near singularities

- near tangencies & corners

Content:

- Main results I+II
- Tri-atomic reactions and soft impact systems

• Near vertical walls (I)

- set up (consider general separable systems)
- The Impact Energy-Momentum diagram
- The Hill region and its foliation
- Return maps
- Main results for case I : near-integrablity of simple impacts
- Some conjectures and numerical simulations
- Near right angled corners (II)
- Summary, open problems

Set up:

$$H = H(\cdot; \epsilon_r, \epsilon_w, q^w, b) = H_{int}(q_1, p_1, q_2, p_2) + \epsilon_r V_r(q_1, q_2) + b \cdot V_b(q - q^w; \epsilon_w)$$

Potential level lines:





Phase portraits (separable dynamics)





symmetry-preserving impacts preserve integrability

 $H = H(\cdot; \epsilon_r, \epsilon_w, q^w, b) = H_{int}(q_1, p_1, q_2, p_2) + \epsilon_r V_r(q_1, q_2) + b \cdot V_b(q - q^w; \epsilon_w)$

 $q^w=(0,q_2)$ (with $\varepsilon_r=0$) preserve separability:



Plan:

- Construct Impact Energy Momentum diagram & relate to Hill regions
- Construct local return maps
- Study effects of small perturbations: deformations in wall shape and small ε_r

Energy momentum bifurcation diagram – smooth dynamics



Impact Energy momentum bifurcation diagram (I-EMBD) separable cases:









I-EMBD for slanted wall:

"tangent zone" dynamics









Poincare map for perpendicular wall:

$$\begin{cases} I' = I\\ \theta' = \theta + \omega_2(I) \cdot (T_1(J) - \Delta t_{travel}(J)) = \theta + 2\pi \frac{\tilde{T}_1(J)}{T_2(I)} \equiv \theta + \Theta(I, J(H, I)) \end{cases}$$

Away from tangency - smooth twist map, with possibly isolated non-twist tori.

Non-twist torus \Rightarrow $\tilde{T}'_1(J) \cdot T'_2(I) \leq 0$ (here occurs inside separatrix)

Near vertical walls (I) : global phase space structure +retrurn maps



I-EMBD

Near –Integrable dynamics:

"Away" from the singularities & degeneracies (tangencies, separatrices, non-twist tori), the return map is smooth and C^r-close to the integrable twist map



THEOREM 2.6. (Smoothness of the return map (9)) Consider a Hamiltonian H of the form Eq. (1) with an S3B integrable structure H_{int} and a regular wall position (Definition 2.3), with $\epsilon_r = \epsilon_w = 0$. Fix $\delta > 0, \rho > 0$, and consider a δ -regular energy level H < b. Then for I in $H_2^{-1}(\mathbb{H}_2^{R,\delta}(H))$, excluding a ρ - interval centered at I_{tan} (so $I \in H_2^{-1}(\mathbb{H}_2^{R,\delta}(H)) \setminus \mathcal{N}_{\rho}(I_{tan}(H))$), the return map $\mathcal{F}_0 : (I, \theta) \to (\bar{I}, \bar{\theta})$ is symplectic and C^r smooth, i.e. $\exists M_r(\rho, \delta) < \infty$ such that $||\Theta(I, J(H, I))||_{C^r} < M_r(\rho, \delta)$. Moreover, the regular set $H_2^{-1}(\mathbb{H}_2^{R,\delta}(H)) \setminus \mathcal{N}_{\rho}(I_{tan}(H))$ on which the return map (9) is C^r smooth is of $\mathcal{O}(1)$ in δ, ρ .

Proof: transverse sections & finite travel times

THEOREM 3.1. Consider a Hamiltonian H of the form Eq. (1) with an S3B integrable structure H_{int} and a regular wall position. Fix $\delta > 0, \rho > 0$, let $\epsilon = (\epsilon_r, \epsilon_w)$ and $\varepsilon = ||\epsilon||$, and consider a δ -regular energy level H < b. Then for $I \in H_2^{-1}(\mathbb{H}_2^{R,\delta}(H)) \setminus \mathcal{N}_{\rho}(I_{tan})$, for all θ , for sufficiently small ε the return map \mathcal{F}_{ϵ} : $(I, \theta) \to (\bar{I}, \bar{\theta})$ is symplectic, C^r smooth and $\varepsilon - C^r$ close to the unperturbed impact return map \mathcal{F}_0 of (9). Namely, for all (I, θ) in this bounded domain, there exists $\varepsilon_0(H, \delta, \rho) > 0$, such that for all $\varepsilon \in [0, \varepsilon_0(H, \delta, \rho))$:

(14)
$$\mathcal{F}_{\epsilon} : \begin{cases} \bar{I} = I + \varepsilon f(I,\theta;\epsilon) \\ \bar{\theta} = \theta + \Theta(I,J(H,I)) + \varepsilon g(I,\theta;\epsilon) \end{cases}$$

with $f, g \ 2\pi - periodic$ in $\theta, f, g \in C^r$.

Proof: transverse sections & finite travel times of

$$\mathcal{F}_{\epsilon} = \Phi_{\epsilon_r}^{[t_{\epsilon}^*, t_{\epsilon}^{**}]} \circ S_{\epsilon_w} \circ \Phi_{\epsilon_r}^{[0, t_{\epsilon}^*]}$$

Near vertical walls (I) : KAM Theory applied to impact systems

COROLLARY 3.2. For fixed H and $\delta, \rho > 0$, consider a circle which is bounded away from separatrices, tangencies and the non-twist set, i.e. I_0 belongs to the closed "good" set $I_0 \in H_2^{-1}(\mathbb{H}_2^{R,\delta}(H)) \setminus (\mathcal{N}_{\rho}(I_{tan}) \cup \mathcal{N}_{\rho}(\mathbf{I}_{NT}(H))) \equiv S_g(H, \delta, \rho)$. Furthermore, assume $\Theta(I_0, J(H, I_0))/2\pi$ is (c, ν) -Diophantine

(16)
$$| \Theta(I_0, J(H, I_0)) - \frac{2\pi m}{n} | > cn^{-\nu - 1} \ \forall m \in \mathbb{Z}, n \in \mathbb{Z}^*$$

where $1 < \nu < \frac{1}{2}(r-1)$. Then, there exists $\varepsilon_1(H, \delta, \rho; c, \nu)$ such that for all $\varepsilon < \varepsilon_1$ there exists a perturbed invariant circle $(I_{\varepsilon}(\theta), \theta)$ with rotation number $\frac{\tilde{T}_1(J(H, I_0))}{T_2(I_0)}$ which is ε/c close to the unperturbed circle $I = I_0$. Furthermore, the same result is valid for small c as long as c is at least of $\mathcal{O}(\sqrt{\varepsilon})$.

Proof: small smooth perturbation of a twist map + show that for small ε trajectories remain in the "good set"- KAM applies

COROLLARY 3.3. Consider a Hamiltonian H of the form Eq. (1) with an S3B integrable structure H_{int} , a regular wall position and assume the integrable impact system has a non-degenerate impact twist. Fix $\delta > 0, \rho > 0$, let $\epsilon = (\epsilon_r, \epsilon_w)$ and $\varepsilon = ||\epsilon||$, and consider a δ -regular energy level H < b. Then, for sufficiently small ε , the complement to the set of all tori I_0 belonging to the energy surface H and satisfying the conditions of Corollary 3.2, namely the set of tori which do not necessarily persist under ε perturbations is of $\mathcal{O}(\sqrt{\varepsilon}, \rho, \delta | \ln \delta |)$.

Proof: Excluding resonances and the complementary to the "good set"- KAM applies

For sufficiently small ϵ most phase space is foliated by KAM tori

Near vertical walls (I) : Perturbation theory for the impact systems



First order approximations to the perturbed twist map: vertical wall

THEOREM 3.5. Consider a Hamiltonian H of the form (1) with an S3B integrable structure H_{int} and a regular wall position, with $\epsilon_w = 0$. Fix $\delta > 0$, $\rho > 0$, and consider a δ -regular energy level H. Then for $I \in H_2^{-1}(\mathbb{H}_2^{R,\delta}(H)) \setminus \mathcal{N}_{\rho}(I_{tan})$, for all θ , for sufficiently small ϵ_r , the function f of the change in I in the return map (14) has the following form:

(18)
$$f(I,\theta;\epsilon_r) = -\frac{1}{\omega_2(I)} \int_0^{T_1(J(I,H))} \left(\frac{\partial V_r}{\partial q_2} p_2\right)_{z_0^{im}(t)} dt + \mathcal{O}(\epsilon_r)$$

$$H = H(\cdot; \epsilon_r, \epsilon_w, q^w, b) = H_{int}(q_1, p_1, q_2, p_2) + \epsilon_r V_r(q_1, q_2) + b \cdot V_b(q - q^w; \epsilon_w)$$

$$\mathcal{F}_{\epsilon} = \Phi_{\epsilon_r}^{[t^*_{\epsilon}, t^{**}_{\epsilon}]} \circ S_{\epsilon_w} \circ \Phi_{\epsilon_r}^{[0, t^*_{\epsilon}]}$$

$$I^* = I(t^*_{\epsilon_r}) = I + \int_0^{t^*_{\epsilon_r}} \{I, H_{int} + \epsilon_r V_r\} \mid_{z_{\epsilon_r}(t)} dt = I + \int_0^{t^*_0} + \int_{t^*_0}^{t^*_{\epsilon_r}} \{I, \epsilon_r V_r\} \mid_{z_{\epsilon_r}(t)} dt$$
$$= I + \epsilon_r \int_0^{t^*_0} \{I, V_r\} \mid_{z^{im}_0(t)} dt + \mathcal{O}(\epsilon_r^2)$$

$$\begin{split} I' &= I(t_{\epsilon_r}^{**}) = I(t_{\epsilon_r}^{*}) + \int_{t_{\epsilon_r}^{*}}^{t_{\epsilon_r}^{**}} \{I, H_{int} + \epsilon_r V_r\} \mid_{z_{\epsilon_r}(t)} dt \\ &= I^* + \int_{t_{\epsilon_r}^{*}}^{t_0^{**}} \{I, \epsilon_r V_r\} \mid_{z_{\epsilon_r}(t)} dt + \int_{t_0^{**}}^{t_{\epsilon_r}^{**}} \{I, \epsilon_r V_r\} \mid_{z_{\epsilon_r}(t)} dt \\ &= I^* + \epsilon_r \int_{t_{\epsilon_r}^{*}}^{t_0^{**}} \{I, V_r\} \mid_{z_0^{im}(t)} dt + \mathcal{O}(\epsilon_r^2) = I^* + \epsilon_r \int_{t_0^{*}}^{t_0^{**}} \{I, V_r\} \mid_{z_0^{im}(t)} dt + \mathcal{O}(\epsilon_r^2). \end{split}$$



 $\mathcal{F}_{\epsilon} : \begin{cases} I' = I + \varepsilon f(I, \theta; \epsilon) \\ \theta' = \theta + \Theta(I, J(H, I)) + \varepsilon g(I, \theta; \epsilon) \end{cases}$

First order approximations of the perturbed twist map

Perpendicular wall with coupling perturbation:

$$f(I,\theta;\epsilon_r) = \frac{1}{\omega_2(I)} \int_0^{\tilde{T}_1(J(I,H))} \left(\frac{\partial V_r}{\partial q_2} \ p_2\right)_{z_0^{im}(t)} dt + \mathcal{O}(\epsilon_r)$$





Theorem: First order approximations of the perturbed twist map (slanted case)

COROLLARY 3.6. For H, ϵ_w and initial conditions $(\tilde{I}, \tilde{\theta})$ which satisfy the assumptions of Theorem 3.1 with r > 4, an impact by a near perpendicular straight wall is equivalent to the system with impact with a perpendicular wall and a small, regular perturbation. Moreover, the form of the change in \tilde{I} due to the wall tilt becomes (see Theorem 3.5):

(28)
$$f(\tilde{I}, \tilde{\theta}; \epsilon_w) = -\frac{1}{\omega_2(\tilde{I})} \int_0^{\tilde{T}_1(\tilde{J})} \left(\left[-V_1'(\tilde{q_1}) + \tilde{q_1} \cdot V_2''(\tilde{q_2}) \right] \tilde{p_2} \right)_{\tilde{z_0}^{im}(t)} dt + \mathcal{O}(\epsilon_w)$$

Near integrable soft steep potentials:

$$H = H(\cdot; \epsilon_r, \epsilon_w, \epsilon_b, q^w, b) = H_{int}(q_1, p_1, q_2, p_2) + \epsilon_r V_r(q_1, q_2) + b \cdot V_b(q; \epsilon_w, \epsilon_b)$$

$$V_{b,poly}(q;\epsilon_w,\epsilon_b) = \frac{\epsilon_b}{q_1 - \epsilon_w Q^w(q_2;\epsilon_w)}$$
$$V_{b,exp}(q;\epsilon_w,\epsilon_b) = \exp\left(-\frac{q_1 - \epsilon_w Q^w(q_2;\epsilon_w)}{\epsilon_b}\right)$$

THEOREM 3.7. Consider a Hamiltonian H of the form (31) with an S3B integrable structure H_{int} , a regular wall position, and a soft billiard potential V_b satisfying conditions I-IV (see appendix B). Fix $\delta > 0, \rho > 0$, let $\epsilon = (\epsilon_r, \epsilon_w, \epsilon_b)$ and $\varepsilon = ||\epsilon||$, and consider a δ -regular energy level H satisfying $H < H_{max}(b)$ (see appendix). Then for $I \in H_2^{-1}(\mathbb{H}_2^{R,\delta}(H)) \setminus \mathcal{N}_{\rho}(I_{tan})$, for all θ , for sufficiently small ε the return map $\mathcal{F}_{\epsilon} : (I, \theta) \to (\overline{I}, \overline{\theta})$ is symplectic, C^r smooth and C^k close to the unperturbed impact return map \mathcal{F}_0 of (9) for any $k \leq r$. Namely, for all (I, θ) in this bounded domain, there exists $\varepsilon_b^k(H, \delta, \rho) > 0$ such that for all $\varepsilon \in [0, \varepsilon_b^k(H, \delta, \rho)), \mathcal{F}_{\epsilon} = \mathcal{F}_0 + o_{C^k}(1)$.

Proof: All reflections are transverse → by Kloc & RK (2014) the return map of the steep soft impact is C^r close to the impact one.

COROLLARY 3.9. There exists $\epsilon_{b,k}(\epsilon_r, \epsilon_w)$ such that for all $\epsilon_b < \epsilon_{b,k}$, under the conditions of Theorem 3.7, the soft impact return map \mathcal{F}_{ϵ} is $\varepsilon - C^k$ close to \mathcal{F}_0 and in the special calculable cases the first order term in ε of the soft impact return map takes the corresponding forms (18), (28) or (30).

For example, we conjecture that if for a given soft potential form the error estimate for C^k closeness as in [30] is of $\mathcal{O}({}^{k+2}\sqrt{\epsilon_b})$, then for $\epsilon_b \leq \mathcal{O}(\epsilon_r^{k+2}, \epsilon_w^{k+2})$ the overall error would be of $\mathcal{O}(\varepsilon)$ as required.

Remark:

errors coming from the steep potential are yet to be studied.



Near vertical walls (I) : Near tangencies - new phenomena



The perturbed twist map for higher dimensions

 $\{p_n = 0, \dot{p_n} < 0\}$

Consider a separable n d.o.f. system + perturbations +(soft) impacts:

 $H = H(\cdot; \epsilon_r, \epsilon_w, q^w, b) = H_{int}(q, p) + \epsilon_r V_r(q; \epsilon_r) + b \cdot V_b(q - q^w; \epsilon_w, \epsilon_b), \ H_{int}(q, p) = \sum_{i=1}^n H_i(q_i, p_i)$

When the wall normal is aligned with one of the axis, e.g.:

$$q^{w} := \{ (q_1, ..., q_n) \in \mathbb{R}^n : q_n = 0 \}$$

The Poincare return map to (near a p.o. transverse to this section)

$$\begin{cases} I' = I\\ \theta' = \theta + \frac{\Omega(I)}{\omega(J)} \cdot (2\pi - \Delta \varphi(J)) \end{cases}$$

$$I = (I_1, ..., I_{n-1}), \theta = (\theta_1, ..., \theta_{n-1}), \Omega(I) = (\omega_1(I_1), ..., \omega_{n-1}(I_{n-1}))$$

$$\Delta \varphi = \omega(J) \cdot \Delta t_{travel}(J) \qquad J = J(H, I) \qquad H_{int}(I, J) = H$$

Perturbations→ KAM, resonances, manifold splittings, Arnold diffusion ...

MAIN MESSAGE: New class of systems to play with!

See: M. Pnueli and VRK, SIAM DS, 2018, to appear

Can now analyze n dof systems of the form:

$$H = H(\cdot; \epsilon_r, \epsilon_w, q^w, b) = H_{int}(q, p) + \epsilon_r V_r(q; \epsilon_r) + b \cdot V_b(q - q^w; \epsilon_w, \epsilon_b)$$

integrable + coupling +

steep potentials close to symmetry–respecting impacts

Rich class of systems, amenable to perturbation theory !

Developed tools:

I-EMBD

Hill region foliations

Perturbative expressions for return maps

Still developing: return maps near tangencies & near separatrices, Fomenko graphs, higher dimensions + more geometries, moving boundaries, more symmetries, slow-fast cases..

Main results I: (M. Pnueli and VRK, SIAM DS, 2018, to appear)

separable Mech. Hamiltonian + C^r smooth coupling + C^r deformation of a vertical wall

$$H_{int}(q_1, p_1, q_2, p_2) + \epsilon_r V_r(q_1, q_2) + b \cdot V_b(q - q^w; \epsilon_w)$$

<u>Result IA:</u> Impact-Energy-Momentum-Bifurcation Diagram → global dynamical behavior of the system other symmetries & symmetric impacts may be similarly studied

Theorem IB: The dynamics is "mostly" near-integrable –

- in most phase space regions it is C^r close to a twist map.

In particular for sufficiently small ϵ KAM theory applies !

Theorem IC:Explicit formula for the perturbation term of the return map[in some cases: small coupling with either perpendicular or slightly tilted straight wall]

Theorem ID:

The same theorems apply for soft billiard potentials* provided the soft potential is sufficiently steep!

$$H_{int}(q_1, p_1, q_2, p_2) + \epsilon_r V_r(q_1, q_2) + b \cdot V_b(q; \epsilon_w, \epsilon_b)$$

e.g.

$$V_{b,poly}(q;\epsilon_w,\epsilon_b) = \frac{\epsilon_b}{q_1 - \epsilon_w Q^w(q_2;\epsilon_w)}$$

$$V_{b,exp}(q;\epsilon_w,\epsilon_b) = \exp\left(-\frac{q_1 - \epsilon_w Q^w(q_2;\epsilon_w)}{\epsilon_b}\right)$$

* By applying results from:

"Smooth Hamiltonian systems with soft impacts"

M. Kloc & V. R-K SIAM J. Appl. Dyn. Syst., 13-3 (2014)

"Billiards: a singular perturbation limit of smooth Hamiltonian flows"

V. Rom-Kedar and D.Turaev, Chaos 22, 026102 (2012)



Content:

- Tri-atomic reactions and soft impact systems
- Near vertical walls (I) :
 - The Impact Energy-Momentum diagram
 - The Hill region and its foliation
 - Return maps and their approximations
 - KAM theory applies
 - Tangencies..
- Near right angle corners (II):

work in progress w W L. Becker, S. Elliott, B. Firester, S. Gonen Cohen & M. Pnueli

- Global dynamics : the Impact Energy-Momentum diagram for 90°, 270° corners
- Return maps
- impact from corners → study of near-integrable symplectic IEM families
- Some conjectures and numerical simulations
- Summary, open problems

Main results II:

L. Becker, S. Elliott, B. Firester, S. Gonen Cohen, M. Pnueli and VRK,

(in writing..).



or more generally, collection of symmetry-preserving impacting surfaces with discontinuous behavior at the corner points.

Main result IIA:

Without coupling :

Get different Interval Exchange Map (IEM) on each level set !

inspired by very interesting results for Billiards w corners:

Zorich 2000, 2006,2018, Dragovich & Radnovic 2014-2018, V.A. Moskvin 2018

Main result IIB:

With coupling:

A new type of "Standard families of IEM"

Near right angle corners (II) : Global dynamics - IEMBD











Symplectic return map to $\Sigma_1 : (I_2, \theta_2) \rightarrow F(I_2, \theta_2)$

• The return time $\tilde{T}_i = T_i - \Delta t_{i-travel}$ to Σ_i depends only on the energy e_i Hence: $\bar{\theta}_2 = \theta_2 + \frac{2\pi}{T_2(I_2)}\tilde{T}_1(I_1) + k(I,\theta_2)\Delta\theta_2^r(I_2)$ for k bounces from the q_2 wall $\bar{\theta}_2 = \theta_2 + \Theta(I) + 2\pi K(I) + \delta_{k(I,\theta_2),K(I)}\Delta\theta_2^r(I_2)$

Where:

$$\begin{split} \Theta(I) &= 2\pi \left\{ \frac{\tilde{T}_1(I_1)}{\tilde{T}_2(I_2)} \right\} \frac{\tilde{T}_2(I_2)}{T_2(I_2)}, \qquad K(I) = \left\lfloor \frac{\tilde{T}_1(I_1)}{\tilde{T}_2(I_2)} \right\rfloor, \\ \Delta \theta_2^r(I_2) &= 2\pi (1 - \frac{\tilde{T}_2(I_2)}{T_2(I_2)}) \end{split}$$

Near corners (II) : Local analysis – return maps - 90°



Where:

$$\Theta(I) = 2\pi \left\{ \frac{\tilde{T}_1(I_1)}{\tilde{T}_2(I_2)} \right\} \frac{\tilde{T}_2(I_2)}{T_2(I_2)}, \qquad K(I) = \left\lfloor \frac{\tilde{T}_1(I_1)}{\tilde{T}_2(I_2)} \right\rfloor,$$
$$\Delta \theta_2^r(I_2) = 2\pi (1 - \frac{\tilde{T}_2(I_2)}{T_2(I_2)})$$



$$k(I,\theta_2) = \begin{cases} K(I) & \theta_2 \in (\theta_2^+(q_2^{wall}, I_2), \theta_2^-(q_2^{wall}, I_2) - \Theta(I)) \\ K(I) + 1 & \theta_2 \in (\theta_2^-(q_2^{wall}, I_2) - \Theta(I), \theta_2^-(q_2^{wall}, I_2)) \end{cases}$$

 $\bar{\theta}_2 = \theta_2 + \Theta(I) + 2\pi K(I) + \delta_{k(I,\theta_2),K(I)} \Delta \theta_2^r(I_2)$

For a fixed level set -

an interval exchange map with two intervals

= rotation on a circle



Near corners (II) : Local analysis – return maps - 270°



1) The travel time between Σ_i s depends on the energy e_i only

2) The gained phase in θ_2 is constant on intervals – it only depends on the number of collisions with the step!

→ Get interval exchange maps!

Near corners (II) : Local analysis – return maps - 270°

 $\bar{\theta}_2 = \begin{cases} \theta_2 + \frac{2\pi}{T_2(I_2)}\tilde{T}_1(I_1) & \text{reflect from right wall} \\ \theta_2 + \frac{2\pi}{T_2(I_2)}T_1(I_1) + k(I,\theta_2)\Delta\theta_2^r(I_2) & \text{reflect k times from upper wall} \end{cases}$









$$\bar{\theta}_2 = \begin{cases} \theta_2 + \frac{2\pi \tilde{T}_1}{T_2} & \text{reflect from right wall} \\ \theta_2 + \frac{2\pi \tilde{T}_1}{T_2} + \frac{2\pi \tilde{T}_2(e_2;q_2^{wall})}{T_2(e_2)} \left\{ \frac{\Delta t_{1-travel}}{\tilde{T}_2} \right\} + 2\pi K & \text{reflect K times from upper wall} \\ \theta_2 + \frac{2\pi \tilde{T}_1}{T_2} + \frac{2\pi \tilde{T}_2(e_2;q_2^{wall})}{T_2(e_2)} \left\{ \frac{\Delta t_{1-travel}}{\tilde{T}_2} \right\} + \Delta \theta_2^r + 2\pi K & \text{reflect K+1 times from upper wall} \end{cases}$$

$$K(e_1, e_2; q_1^{wall}, q_2^{wall}) = \left\lfloor \frac{T_1(e_1) - \tilde{T}_1(e_1; q_1^{wall})}{\tilde{T}_2(e_2; q_2^{wall})} \right\rfloor = \left\lfloor \frac{\Delta t_{1-travel}(e_1, q_1^{wall})}{\tilde{T}_2(e_2; q_2^{wall})} \right\rfloor$$



$$\lambda = \left(\frac{2\pi\tilde{T}_2}{T_2(e_2)} \left\{\frac{\Delta t_{1-travel}}{\tilde{T}_2}\right\}, \Delta\theta_2^r, 2\pi - \Delta\theta_2^r - \frac{2\pi\tilde{T}_2}{T_2(e_2)} \left\{\frac{\Delta t_{1-travel}}{\tilde{T}_2}\right\}\right)$$



 $\Pi_0 = [ABCDE]$

Π₁ = [EACBD]

$$\bar{\theta}_2 = \begin{cases} \theta_2 + \frac{2\pi \tilde{T}_1}{T_2} & \text{reflect from right wall} \\ \theta_2 + \frac{2\pi \tilde{T}_1}{T_2} + \frac{2\pi \tilde{T}_2(e_2;q_2^{wall})}{T_2(e_2)} \left\{ \frac{\Delta t_{1-travel}}{\tilde{T}_2} \right\} + 2\pi K & \text{reflect K times from upper wall} \\ \theta_2 + \frac{2\pi \tilde{T}_1}{T_2} + \frac{2\pi \tilde{T}_2(e_2;q_2^{wall})}{T_2(e_2)} \left\{ \frac{\Delta t_{1-travel}}{\tilde{T}_2} \right\} + \Delta \theta_2^r + 2\pi K & \text{reflect K+1 times from upper wall} \end{cases}$$

In the impact region, the unperturbed map is NOT conjugate to a rotation!

It is conjugate to motion on torus with at least 2 handles!

see the IEM works and works on billiards w corners – Zorich 2000-2018, Dragovich & Radnovic 2014, V.A. Moskvin 2018

$$\lambda = \left(\frac{2\pi\tilde{T}_2}{T_2(e_2)} \left\{\frac{\bigtriangleup t_{1-travel}}{\tilde{T}_2}\right\}, \bigtriangleup \theta_2^r, 2\pi - \bigtriangleup \theta_2^r - \frac{2\pi\tilde{T}_2}{T_2(e_2)} \left\{\frac{\bigtriangleup t_{1-travel}}{\tilde{T}_2}\right\}\right)$$



 $\Pi_0 = [ABCDE]$

 $\Pi_1 = [EACBD]$

Here: the size and number of interval changes on an energy surface:



Small coupling/deformations → Symplectic perturbation of FIEM transformations:

$$\theta' = \theta + \omega_{\alpha}(I) + \epsilon g(\theta), \qquad \theta \in \mathcal{J}_{\alpha}(I)$$
$$I' = I + \epsilon f(\theta')$$

E.g. : The Standard Map as a FIEM with N=2-intervals

$$g(\theta) = 0, \quad f(\theta') = \sin \theta'$$

$$\omega_{\alpha}(I) = \begin{cases} I & \theta \in [0, 2\pi - I] \\ I - 2\pi & \theta \in [2\pi - I, 2\pi) \end{cases}$$

Simulations: d=5, different permutations, e.g

$$g(\theta) = 0,$$

$$f(\theta') = \sin \theta'$$

$$\omega_{\alpha}(I) = \Omega \lambda_{\alpha}(I)$$

$$\lambda_{\alpha}(I) = \lambda_{\alpha}^{0} + \beta \lambda_{\alpha}^{1} \sin(I)$$

$$\Omega = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 1 \\ 0 & -1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 \\ -1 & -1 & -1 & -1 & 0 \end{pmatrix}$$







ABCDE to EDCBA ϵ = 0.1 no of iterations= 10000



4.5

4

3.5

2.5









Near corners (II) :Numerical return map for the perturbed step dynamics





Summary:

We extend the existing perturbation theory to a much larger class of problems

We show that new phenomena emerge near singularities – tangencies & corners

We construct FIEM – families of interval exchange maps

their unperturbed dynamics is NOT the standard Liuoville-Arnold integrable ! Signal? Applications?



References:

M. Pnueli & V. RK, On near integrability of some impact systems, SIAM DS, 2018, to appear. arXiv preprint arXiv:1803.10987, 2018

Lerman & RK A saddle in a corner - model of collinear chemical reactions, *SIAM J. Appl. Dyn. Syst.*, Vol. 11, No. 1, pp. 416–446, 2012

Kloc & RK Soft impacts theory and multi-dimensional chem reactions: *SIAM J. Appl. Dyn. Syst.*, 13-3 (2014), pp. 1033-1059

Soft Billiards:

Turaev & RK: Elliptic orbits near tangencies -Nonlinearity 11(3), 1998 Islands near tangent periodic orbits - Physica D, 130 1999 Effects of Corners, J. Stat Phys, 112, 2003 Summary and review, Chaos, 2012

Rapoport, RK & Turaev : Higher dimensional closeness theorems and error estimates, Com. Math. Phys 07. Stability in high dimensional steep repelling potentials, Com. Math. Phys 08

Rapoport & RK: Islands in 3-dim soft dispersing billiards, Chaos 06. Scattering by steep potentials, Phys Rev E 08.

On some nearly separable impact systems - Talk by Vered Rom-Kedar

Lecture notes (Ori S. Katz)

October 23, 2018

Abstract

Near-integrability is usually associated with smooth small perturbations of smooth integrable systems. We show that studying integrable mechanical Hamiltonian flows with impacts that respect the symmetries of the integrable structure provide an additional rich class of non-smooth systems that can be studied by perturbation methods. Moreover, the analysis can be extended to systems with soft steep potentials that limit to the impact systems. For example, for some of these systems, we show that KAM theory may be applied, proving that for a large portion of phase space the perturbed motion is conjugate to rotations on a torus [1]. On the other hand, other simple impact systems have inherently non-rotational motion – we show cases in which the motion is conjugate to geodesic flow on a flat torus with several handles [2].

[1] M. Pnueli & V. Rom-Kedar "On near integrability of some impact systems", SIAM-DS, 2018 to appear.

[2] L. Becker, S. Elliott, B. Firester, S. Gonen Cohen, M. Pnueli & V. Rom-Kedar, in preparation.

1 Lecture notes

Work by M. Pnueli and V. Rom-Kedar, with the ISSI team: Becker, Elliot, Firester and Gonen Cohen.

Impact systems - particles moving in a domain with a Hamiltonian vector field, and a boundary with elastic reflections.

Soft impact systems - at the boundary, instead of a rigid wall there is a very steep potential.

Why do we care about these systems? There are very few systems in which we know how initial conditions develop in a general system. We know about integrable systems, and slow-fast systems. Billiards, soft billiards and impact systems provide a widening of the classes of systems for which we can gain some global knowledge of the phase space.

Initial motivation - chemical reactions. The classical approximation (Bohn-Oppenheimer approximation) produces a 3-body problem, i.e. the classical dynamics is chaotic.

Transition State Theory - reduce to 1D dynamics.

Tri-atomic co-linear reactions - the adiabatic approximation produces a system that can be written as a 2 degree of freedom system. This reduced system, in mass weighted Jacobi coordinates, is a type of impact system, with boundaries with a very steep potential and a bulk with a non-steep potential. This is a general property of molecular dynamics, the steep potential related to the repulsion between atoms when they are very close together.

This motivated the "A saddle in a corner" work, done with L. Lerman. It is a model with a steep potential along a corner similar to a billiard in a corner, and a saddle point potential inside the corner. This simple model produces trajectories similar to those gained by more involved models, but it is simple enough to derive some global properties.

Reflections theorem - an analogy between a steep potential and an impact system.

One type of qualitative behavior is a derivation of when does TST work - when the unstable manifold does not tangle back. In this simple model, it is possible to give geometric criteria. This qualitative understanding is difficult to get from general potentials.

Another qualitative result from the analogy between a steep potential and an impact system - can stable triatomic periodic configurations emerge? Kloc and RK - 2014. The answer is yes.

Backing up to look at simpler problems, we next asked, when can we obtain nearly integrable impact systems? A mechanical example - a mass in a square box connected by springs to the sides. This is a separable, 2 degree of freedom impact system. To add impacts, we can add a narrow third dimension so that when the mass hits the vertical wall there is an impact. If the impact wall is completely vertical, the system is still completely separable, but it is no longer smooth. Perturbing the system in various ways - non-vertical wall, non-perfect springs, etc. how do we analyze this system? It's not a smooth system, so naively KAM theory would not work. Thus, we consider a 2D impact system with a Hamiltonian with potential and a wall. If the impact wall respects the symmetry of the underlying potential, the system remains separable.

$$H = H_{int} (q_1, p_1, q_2, p_2) + \epsilon_r V_r (q_1, q_2) + b \cdot V_b (q - q^b; \epsilon_w)$$

where H_{int} is an integrable hamiltonian, V_r is the coupling between the two degrees of freedom and V_b is the impact potential.

Taking $\epsilon_r = 0$, it turns out that symmetry-preserving impacts preserve integrability.

What happens when you perturb such a system?

The projection tool we use is the energy momentum bifurcation diagram, x axis is H and the y axis is the momentum I. So a vertical line on the diagram corresponds to the energy surface upon which the dynamics occur and a single regular point corresponds to a regular level set of the constants of motion, which can be, in the compact case, a torus or several tori. In the considered case, one of the degrees of freedom has a double-well potential, and there is a separatrix on the diagram describing the transition from two separated components of the level set to one connected component.

Adding a wall, can plot the impact energy momentum bifurcation diagram. In the separable cases (perpendicular wall), there will be lines of tangency dividing the diagram into an impact regime and a non-impact regime. When the wall isn't perpendicular, the line of tangency blows up into a region. There is still a region of non-impact tori and a region of regular impact tori, but this time there is a region of tangency.

To see what happens, we draw a Poincare map. In the separable case, the map can be explicitly written.

Also, when you are away from the tangency, this map is a smooth twist map, with possibly isolated non-twist tori, even when impacts occur.

When adding a perturbation to this map, obtain a perturbed twist map - this claim can be proven! Need to show that the perturbed map is close to the non-perturbed one. Thus, two theorems are formulated and proven about the smoothness of the return map. As soon as this is achieved, KAM can be implemented and shown to hold in this system. Moreover, we show that for a small enough ϵ , most of phase space is foliated by KAM tori. Moreover, we can find an analytic formula for the perturbation of the twist map by use of a Melnikov-type calculation, showing that perturbed orbits are close to un-perturbed ones far from the collision, and near the collision there is a weak coupling.

Indeed, there is a nice agreement between the analysis and numerics.

What if we switch the wall to a steep potential - soft impact systems?

We can show that it will work the same way.

What happens near the tangency? There are very peculiar orbits that are still being studied. This could be the new ingredient that emerges from impact systems.

What if we add degrees of freedom - higher dimensions d = n?

The return map can be written in the separable case, to obtain 2n - 2 return equations. Would KAM be applicable? Arnold diffusion? This is TBD.

Main message - this is a rich class of systems that is amenable to perturbation theory of the form

 $H = H_{int}(q, p) + \epsilon_r V_r(q) + b \cdot V_b(q - q^b; \epsilon_w)$

Near right-angle corners: work with L. Becker, S. Elliott, B. Firester, S. Gonen Cohen, M. Pnueli and VRK (in preparation).

Consider a mass in a 2D square connected by aligned springs to the walls, with a corner or a step. If the step is aligned to the axes, the separability is not broken.

Without coupling, we get different interval exchange maps (IEM) on each level set. With coupling, obtain a new type of standard families of IEM.

Understanding the system, we can differentiate between 90 degree corners and 270 degree corners.

90 degree system - The return time depends on the energy in each degree of freedom. Hence we obtain an IEM with two intervals - this is equivalent to a rotation (on a smaller torus) - therefore adding perturbation we'd expect to see similar behavior (TBD).

270 degree system (step) - There are a few options. Below the step, the travel time can depend only on the energy in the first degree of freedom times the frequency in the second degree of freedom. Above the step, the gained phase depends only on the number of collisions with the step. Thus we obtain three intervals. It's a non-trivial map, meaning that for most of the length of these interval, we will get minimal dynamics. There are works that show that these IEM can be embedded onto barriers in action-angle coordinates.

This means that in the impact regime, the return map is not conjugate to a rotation but to motion on a torus with at least two handles. Can ask, is this integrable or not? Energy is conserved, but dynamics are not on Liouville tori. Here, the size and number of interval exchanges change with energy level sets.

Adding small coupling or deformations, this is a symplectic perturbation of FIEM (families of IEM) transformations.

The question we ask and have not yet answered is, do we get invariant curves similar to KAM?

2 Questions:

- Did you consider chemical reaction with transfer of electron instead of atoms, granting a limit of one neglibible mass? No, this would be a great problem, something to be done.

- Is it possible to find acceleration modes? Or would you need a vibration of the walls? Energy is conserved so there can be no acceleration.